A mechanism-based plastic model to simulate the mechanical properties in nanostructured bimodal metals

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Abstract Engineering a bimodal grain size distribution in nanostructured materials has been proved to effectively achieve both higher strength and higher ductility. In these materials, large grains provide hardening ability and small grains provide larger yield stress. Accounting for the contributions of microcracks which nucleate in the nano/ultrafine grained phase and stop at the boundary of large grains during the plastic deformation, a mechanism-based plastic model is developed to describe the strength and ductility of the bimodal metals. The strain-based Weibull probability distribution function is utilized to predict the failure behavior of the bimodal metals. With the aid of the modified mean field approach, the stress–strain relationship can be derived by combining the constitutive relations of the nano/ultrafine grained phase and the coarse grained phase. Numerical results show that the proposed model can completely describe the mechanical properties of the bimodal metals, including yield strength, strain hardening and uniform elongation. The predictions are in good agreement with the experimental results. These results will benefit the optimization of both strength and ductility by controlling constituent fractions and the size of the microstructures in materials.

Keywords Bimodal grain size distribution, Strength, Strain hardening; Ductility, Weibull distribution

1. Introduction

Nanostructured and ultrafine-grained metallic materials have been observed to perform outstanding physical and mechanical properties. One of the most remarkable improvement is the superior mechanical strength compared to those of corresponding coarse-grained counterparts [1]. Therefore, these materials have been of significant interest and the key importance in designing lighter and stronger structures. So far, there have been several strategies to obtain the higher strengthening materials, including refining grain size, solid solution alloying and plastic straining [2], but these materials perform the disappointingly low tensile ductility. Due to this fact, the simultaneously higher strength and ductility in metals and alloys are expected and have emerged as the essentially challenging issue in the application of the nanostructured metals. In the past ten years, several alternative approaches are addressed to achieve the higher strength with keeping the high ductility, such as by generating the internal boundaries such as nanotwins in polycrystalline metals [3], or mixing the various sizes of microstructures in nanostructured materials [4-5].

The bimodal grain size distributions in nanostructured metals/alloys, which is considered as an effective approach to obtain the higher strength with good ductility, were first studied experimentally by Wang et al [4] and Tellkamp et al. [6] respectively. Their observations showed that such kind of nanostructured metals/alloys have higher strength and high ductility simultaneously. After these pioneering works, the subsequent various experiments and theoretical studies are carried out to investigate the mechanical performance in bimodal nanostructured metals and alloys [7-9]. These experiments demonstrated that the nanograins or ultrafine grains contribute to the higher strength and the higher ductility is attributed to the coarse grains. For the fracture in bimodal metals/alloys, there exist some explanations to shed some lights into the possible mechanism of failure. The cavitations in nanograin/ultrafine phase, necking in coarse grains and shear localization are responsible for the fracture in bimodal metals [10-12]. Besides of that, the cavitations and microcracks play an important role in the improved ductility of the bimodal metals/alloys, which have been indentified further by the recent experiments [13]. The predictions of mechanical behaviors in bimodal metals/alloys have become a key issue to optimize the grain size distribution and the volume fraction of continents in bimodal metals/alloys for desiring the high strength and high ductility. So far, there are several works to develop the theoretical model for predicting the constitutive behavior and the failure properties of bimodal metals/alloys [14-15].

It has been demonstrated in experimental observations of tensile deformation in bimodal materials that the nanoscale voids or nano/microcracks lead to the modification of stress and strain for the plastic deformation. The objective of the present paper is to introduce the mechanism-based plastic model for bimodal metals in which the impacts of the microcracks generated during plastic deformation in bimodal materials on the mechanical properties are accounted for [16]. The bimodal copper is selected as an example to predict the corresponding mechanical behavior of bimodal metals. The weibull probability distribution of nan/microcracks is analyzed in the simulations. Numerical results show that the developed plastic model of bimodal metals can describe the mechanical properties of bimodal copper completely.

2. A Set Up of Model

The nanostructured metal with bimodal grain size distribution is considered as the composite metals consisting of the nanograined matrix phase and the course grained phase, as shown in Fig. 1. Since the grain boundaries have great contribution on the mechanical properties of nanocrystalline materials, the strain gradient in GBDPZs are involved in the proposed model to capture the effects of grain boundaries on the plastic deformation. Therefore, the mechanism-based strain gradient plasticity [17] is adopted here to describe the stress-strain response in each constituent of bimodal metals. A summary of the formulation is provided in the following. The strain rate $\dot{\boldsymbol{\varepsilon}}$ can be decomposed into its elastic and plastic parts,

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{\mathrm{e}} + \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} \tag{1}$$

The elastic strain rate is obtained from the stress rate in the linear elastic relation as

$$\dot{\boldsymbol{\varepsilon}}^{\mathrm{e}} = \mathbf{M} : \dot{\boldsymbol{\sigma}} \tag{2}$$

where $\mathbf{M}$ is the elastic compliance tensor. The plastic strain rate is proportional to the deviatoric stress $\boldsymbol{\sigma}'$ based on the conventional J2-flow theory of plasticity, given as

$$\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \frac{3\dot{\varepsilon}^{\mathrm{p}}}{2\sigma_{\mathrm{e}}}\boldsymbol{\sigma}' \tag{3}$$

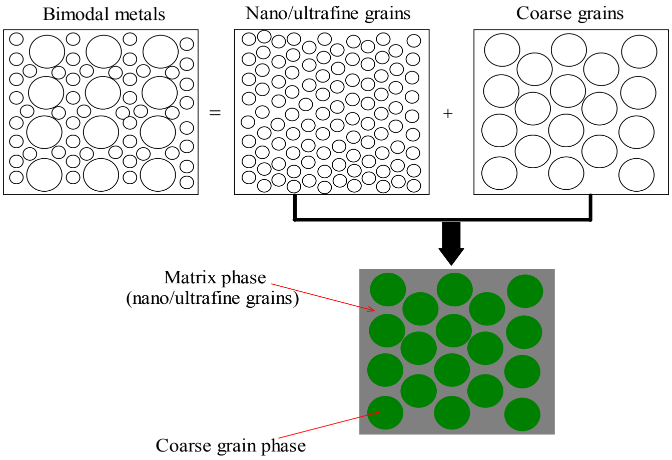

Fig. 1 Schematic drawings of bimodal grain size distributions in polycrystalline materials with assumption of the composite mixture model.

Here, $\sigma'_{ij} = \sigma_{ij} - \sigma_{kk}\delta_{ij}/3$ and $\sigma_e = \sqrt{3\sigma'_{ij}\sigma'_{ij}/2}$ is the von Mises equivalent stress. $\dot{\varepsilon}^p$ is the equivalent plastic strain rate which is determined by

$$\dot{\varepsilon}^p = \dot{\varepsilon}\left[\frac{\sigma_e}{\sigma_{flow}}\right]^{m_0} \tag{4}$$

in which $\dot{\varepsilon} = \sqrt{2\dot{\varepsilon}'_{ij}\dot{\varepsilon}'_{ij}/3}$ is the equivalent strain rate and $\dot{\varepsilon}'_{ij} = \dot{\varepsilon}_{ij} - \dot{\varepsilon}_{kk}\delta_{ij}/3$. m_0 is the rate-sensitivity exponent and σ_{flow} is the flow stress which will be addressed in the coming subsections for coarse grain and nano/ultrafine grains respectively. Eqs. (2)-(4) then establish the triaxial constitutive relation for the constituents in bimodal metals.

In the coarse grains, the surface-to-volume ratio of the grain boundaries is low enough to neglect its contribution on the plastic deformation. The primate deformation mechanism is dominated by the intragrain dislocation-mediated interaction which can be described by the Taylor evolution law. Thus the flow stress of the coarse grain can be expressed as

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b\sqrt{\rho} + \sigma_b \tag{5}$$

Here, α , μ and M are the empirical constant, the shear modulus and the Taylor factor, respectively. σ_0 is the lattice friction stress and σ_b represents the back stress . ρ denotes the density of dislocations in grains which can be determined by the Kocks-Mecking's model [40]. According to Kocks and Mecking's model, the density of dislocations in the crystal interior obeys the evolution law with plastic strain, which allows for competition between accumulation and annihilation by dynamic recovery [18].

For the flow stress in the nano/ultrafined grains phase, the isotropic strain hardening is involved in the flow stress that is in consistency with the one in coarse grains described by Kocks-Mecking model, while the back stress with respect to the kinematic strain hardening is excluded in the nano/ultrafine grains phase. Then, the flow stress of the matrix phase can be expressed by

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b\sqrt{\rho_I + \rho_{GB}} \tag{6}$$

in which the Taylor term in the flow stress is relevant to the dislocation densities in crystal interior and the GBDPZ. The density of dislocations in the GBDPZ can be expressed by

$$\rho_{GB} = \frac{n^{GB}\lambda^{GB}}{V_{Cell}} = k^{GB}\frac{\eta^{GB}}{b} \tag{7}$$

Here, $k^{GB} = 6d_{GBDPZ} / \phi^{GB} d_G$.

2.1. Impact of nano/microcracks

As the appearance of microcracks indicates, the number of dislocations stopped at the grain boundaries or around the cracks is increased. These dislocations pile up along the grain boundaries, impeding the movement of dislocations and ultimately resulting in back stress effects that must be taken into account during the plastic deformation in the nano/ultrafine-grained phase. Thus, the constitutive relation of the nano-grained phase will involve the back stress term in the flow stress expression. The flow stress in this phase is rewritten as

$$\sigma_{flow} = \sigma_0 + M\alpha\mu b\sqrt{\rho_I + \rho_{GB}} + \sigma_b^*, \tag{8}$$

where σ_b^* is the microcrack-induced back stress. The microcrack-matrix-effective-medium approach is utilized here to model the overall stress and strain in the nano/ultrafine-grained phase of the bimodal metals. The representative volume element (RVE) is often applied to account for the crack orientation statistics in the composite mechanics. The RVE boundary is subjected to tractions in equilibrium with a uniform overall stress of σ^∞ and the average strain in a solid with microcracks is consistent with regular and singular parts as

$$\bar{\boldsymbol{\varepsilon}} = \bar{\boldsymbol{\varepsilon}}^{\mathbf{m}} + \bar{\boldsymbol{\varepsilon}}^{\mathbf{c}}, \tag{9}$$

where $\bar{\boldsymbol{\varepsilon}}^{\mathbf{m}}$ and $\bar{\boldsymbol{\varepsilon}}^{\mathbf{c}}$ denote the matrix strain averaged over the RVE and the microcrack-induced variations in the overall average strain, respectively. If the matrix satisfies to be linear elastic, the matrix strain can be written as $\bar{\boldsymbol{\varepsilon}}^{\mathbf{m}} = \mathbf{M}^{\mathbf{m}} : \boldsymbol{\sigma}^\infty$. Because the microcracks generated during the plastic deformation of the bimodal metals are supposed to be parallel, the corresponding effective moduli are as follows:

$$E_1 = E_0[1 + \frac{16(1-v_0^2)}{3}\rho]^{-1}; G_{12} = G_0[1 + \frac{8(1+v_0)}{3(1-v_0/2)}\rho]^{-1}. \tag{10}$$

Please note from Eq.(15) that the effective moduli of the bimodal metals are associated with the density of microcracks in the materials. Experiments have revealed that the number of microcracks in the bimodal metals increased during the plastic deformation, suggesting that the density of microcracks in the bimodal metals is sensitive to the applied stress or strain. From this perspective, the strain-based Weibull distribution function with respect to the plastic strain is adopted here to character the number of microcracks. Thus the density of microcracks can be expressed as following

$$\rho = \rho_0 P(f_W) = \rho_0(1 - f_W(\varepsilon_p)) \tag{11}$$

Here, ρ_0 is a constant; $f_W(\varepsilon_p) = \exp(-(\varepsilon_p/\varepsilon_0)^m)$ is the strain-based Weibull distribution function in which ε_0 is the reference strain and m is the Weibull modulus.

2.2. Composite model

The composite model derived from the modified mean-field approach involves the Hill's recognition of a weakening constraint power for plastic deformation [19]. However, the flow stress in the following derivation is substituted by those in the nano/ultrafine-grained phase and the coarse-grained phase, respectively, both of which will be derived in the next section. Thus, the secant Young's modulus and secant Poisson ratio of the ith phase can be expressed by

$$E^{S(i)} = \frac{E^{(i)}}{1+\dfrac{E^{(i)}\varepsilon^{(i)}}{\sigma_{flow}^{(i)}}\left(\dfrac{\sigma_{11}^{(i)}}{\sigma_{flow}^{(i)}}\right)^{m_0-1}}, v^{S(i)} = \frac{1}{2}-\left(\frac{1}{2}-v^{(i)}\frac{E^{S(i)}}{E^{(i)}}\right) \quad , \tag{12}$$

Throughout this paper the matrix will be indicated as phase 0 and coarse grains as phase 1. $E^{(i)}$ and $v^{(i)}$ denote the Young's modulus and the Poisson's ratio of the ith phase, respectively. The corresponding secant bulk and shear moduli of the ith phase are taken to satisfy the isotropic relations as $k^{S(i)} = E^{S(i)}/[3(1-2v^{S(i)})], \mu^{S(i)} = E^{S(i)}/[2(1+v^{S(i)})]$, respectively. Suppose that the composite is subjected to a boundary-displacement with a uniform strain $\bar{\boldsymbol{\varepsilon}}$, the relationship between the hydrostatic and deviatoric strains of the constituent phases and those of the composite are as follows [19]:

$$\begin{aligned}
\varepsilon_{kk}^{(0)} &= \frac{\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk}, \varepsilon_{ij}^{(0)\prime} = \frac{\beta_0^s(\mu_1-\mu_0^s)}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\bar{\varepsilon}_{ij}' - \frac{c_1\beta_0^s\mu_1}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\varepsilon_{ij}^{p(1)} \\
\varepsilon_{kk}^{(1)} &= \frac{\kappa_0}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk}, \varepsilon_{ij}^{(1)\prime} = \frac{\mu_0^s}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\bar{\varepsilon}_{ij}' + \frac{c_0\beta_0^s\mu_1}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\varepsilon_{ij}^{p(1)}
\end{aligned} \quad , \tag{13}$$

where the mean stress components of the matrix phase and inclusions are given by

$$\begin{aligned}
\sigma_{kk}^{(1)} &= 3\kappa_0\frac{\kappa_1}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk}, \sigma_{ij}^{(1)\prime} = \frac{2\mu_0^s\mu_1[\bar{\varepsilon}_{ij}'-(1-c_0\beta_0^s)\varepsilon_{ij}^{p(1)}]}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s} \\
\sigma_{kk}^{(0)} &= 3\kappa_0\frac{\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk}, \sigma_{ij}^{(0)\prime} = \frac{2\mu_0^s\{[\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s]\bar{\varepsilon}_{ij}'-c_1\beta_0^s\mu_1\varepsilon_{ij}^{p(1)}\}}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}
\end{aligned} . \tag{14}$$

Here, f_i is the volume fraction of the ith phase and α and β are the components of Eshelby's tensor for spherical inclusions, as follows:

$$S_0^s = (\alpha_0^s, \beta_0^s), with\ \alpha_0^s = \frac{1+v_0^s}{3(1-v_0^s)}, \beta_0^s = \frac{2(4-5v_0^s)}{15(1-v_0^s)} . \tag{15}$$

Therefore, the dilatational and deviatoric stresses and strains of the composite are connected by

$$\begin{aligned}
\bar{\sigma}_{kk} &= 3\kappa_0\left[1+\frac{c_1(\kappa_1-\kappa_0)}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\right]\bar{\varepsilon}_{kk}, \\
\bar{\sigma}_{ij}' &= 2\mu_0^s\left\{\left[1+\frac{c_1(\mu_1-\mu_0^s)}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\right]\bar{\varepsilon}_{ij}' - \frac{c_1\mu_1}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\varepsilon_{ij}^{p(1)}\right\}
\end{aligned} . \tag{16}$$

To get an accurate description of the grain size-dependent local interaction and behavior in each phase, the grain size statistical distribution is frequently used to characterize the grain size distribution. Here, the grain size distribution in each phase is supposed to follow a Rayleigh distribution with one parameter, instead of the log-normal distribution, for simplicity [20].

3. Numerical results and discussion

We now apply the developed models to predict the mechanical and failure behaviors of bimodal coppers, and then make comparisons with experimental results of bimodal coppers [4]. In the proposed composite mixture model, the matrix phase and coarse grain phase have equal elastic properties. These and other material parameters used in calculation are adopted in Ref [21]. For the sake of predicting the stress-strain relation of bimodal copper, the constitutive behavior in the matrix phase and coarse grain phase must be captured firstly. With the aid of the proposed constitutive relations, the stress-strain curves of matrix phase with average grain size as 300nm and coarse grain phase with mean grain size as 2μm are given in Fig.2a and Fig.2b respectively, by adopting the corresponding parameters. The corresponding experimental results are also plotted in Fig.2. Due to that the strain gradient is involved in the ultrafine or nanograins phase to describe the contribution of grain boundaries on the deformation mechanism, a reasonable value of strain gradient is provided to fit the experimental data. Note that the prediction can be in good accord with the measurements shown as in Fig.2a. For the coarse grain phase, the isotropic and kinetic strain hardening are both taken into account in the proposed constitutive relation and the calculated results can be agreeable very well with the experimental results (Seen in Fig.2b). After indentifying the constitutive relation in matrix phase and coarse grain phase, we then can simulate the stress-strain response in the framework of the proposed composite model involving the contributions of the microcracks. Fig.3 plots the predicted results based on the proposed model and the experimental data for bimodal copper are also reproduced in the figure. Here, the initial crack density ρ_0 is given as 0.04 and the Weibull modulus m as 10. It can be clearly noticed that the proposed model can capture very well the mechanical behavior in bimodal copper, the agreement between the simulations and the experiments is quite good not only in the yield stress but also in the strain hardening and the elongation at the ultimate strength.

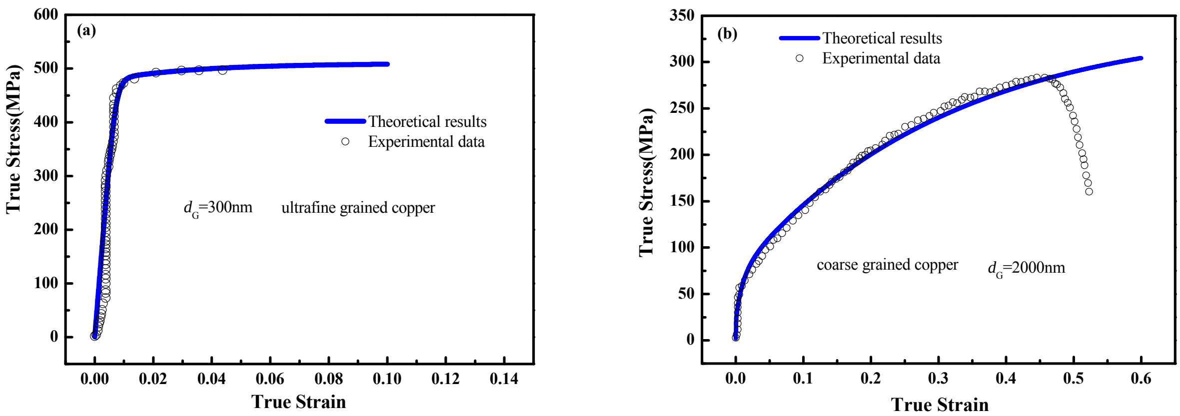

Fig. 2 Comparison of the stress-strain relationship between the experiments and theoretical results of coppers for the ultrafine/nanograins and the coarse grains

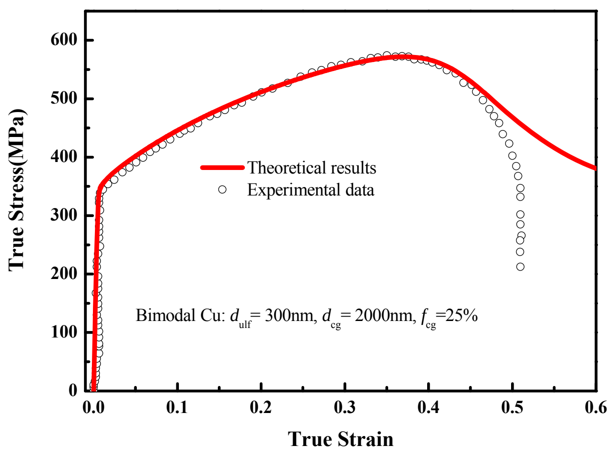

Fig. 3 Comparison of the stress-strain relationship between theoretical results and experiments for the bimodal Cu[8]

Owing to that the matrix grain dominates the high strength of the bimodal coppers and the inhomogeneous microstructures induces various mechanisms of strain hardening, we then further examined the dependence of the volume fraction of coarse grains on the mechanical response in bimodal copper. we plot the strength vs. uniform elongation with dependence of the volume fraction of coarse grains for the Weibull modulus as 3, 6 and 12 in Fig.4. It is worth to note from the figure that the strengths, including yield strength and ultimate strength, is weakened while the ductility is improved with the increment of the volume fraction of coarse grains. For the various Weibull modulus, the ductility increases with the increment of the Weibull modulus, and the slope of the curves for three different Weibull modulus are quite different with each other. It is also interesting to find from Fig.8 that the yield strength is independent on the Weibull modulus while the ultimate strength becomes smaller with decreasing the Weibull modulus.

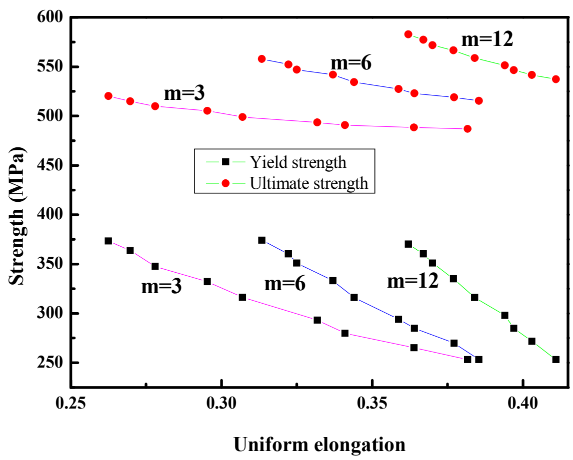

Fig. 4 Relationship between the strength and uniform elongation with different Weibull modulus for bimodal copper (d_{ulf}= 300nm, d_{cg}= 2000nm)

We further plot the curves of failure probability varied with the failure strain from the strain-based Weibull distribution function for the nanograined copper, coarse grained copper as well as bimodal coppers in Fig.5a. Inspired by the experimental observations, the characteristic strain ε_0 is adopted approximately as the measured uniform elongation. The Weibull modulus for the coarse grains and nano grains are determined by fitting the experimental results and the ones for bimodal cases are obtained by comparing with experiments. It can be found from the figure that the curves of bimodal cases are all located in the region surrounded by the curves of nanograins and coarse grains. The curves of bimodal copper with volume fraction of coarse grain as 45% and 83% in Li's measurements [9] are close to the one of the nano grains. It means that the failure properties of these two cases perform in an obvious brittleness comparable with nanocrystalline metals. The curve of the bimodal copper achieved by Wang et al [4], however, approaches the one of the coarse grains as well as the one with coarse grain fractions as 98% [9]. Under the same reference strain, the variability of the failure strain with a large Weibull modulus is less than the one with a small Weibull modulus, as shown in Fig. 9b. It means that, suppose the reference strain in the bimodal metal of $f_c = 0.45$ to be 30%, the limited measurements of corresponding case in Ref.[9] can be included in the reasonable failure probability which is determined by the sufficient data of measured samples.

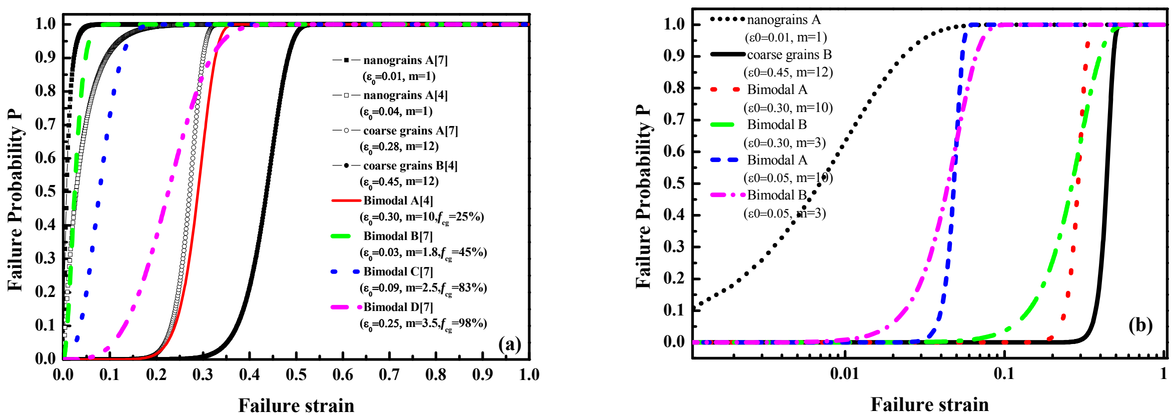

Fig. 5 The failure probability varied with failure strain with different Weibull modulus and a given volume fraction of coarse grain in bimodal copper.

4. Conclusion

In this paper, a micromechanics-based model, which has been developed in the previous authors' work, is introduced to investigate the mechanical behaviors of polycrystalline coppers with bimodal grain size distribution, accounting for the microcracks generated during plastic deformation.. Because of the appearance of the microcracks in the bimodal metals, the local mechanical properties are modified completely. After indentifying the related parameters in the developed model, the stress-strain response of the bimodal copper are predicted to make a comparison with the corresponding experimental results. The present numerical results reveal that the proposed micromechanical model can be utilized to describe the mechanical behavior of bimodal metals completely and successfully and to be expected to predict the mechanical properties such as the yield stress and ductility. The predictions based on the proposed model are agreeable very well with the experimental data of bimodal copper. The results with respect to the Weibull modulus of microcrack density suggest that the bimodal metals will have good ductility with higher Weibull modulus which can be considered to be associated with the microstructures in the materials. The results in this paper will shed some lights on optimizing the distribution of microstructures and the grain size in polycrystalline materials to promise the achievement of higher strength and higher ductility in polycrstal metals or alloys.

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